A General Multi-objective Force Field Optimization Framework and its Application to the Design of Reactive Force Fields for Silicon Carbide

ReaxFF force field file format

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1. GENERAL

1	p(boc_1)	Overcoordination parameter
2	p(boc_2)	Overcoordination parameter
3	p(coa_2)	Valency angle conjugation parameter
4	gp_3	Triple bond stabilization parameter
5	gp_4	Triple bond stabilization parameter
6	p(lp_3)	C2-correction
7	p($ovun_6$)	Undercoordination parameter
8	gp_7	Triple bond stabilization parameter
9	p($ovun_7$)	Undercoordination parameter
10	p($ovun_8$)	Undercoordination parameter
11	gp_{10}	Triple bond stabilization energy
12	nonb_low	Lower Taper-radius
13	nonb_cut	Upper Taper-radius
14	n.u.	
15	p(val_6)	Valency undercoordination
16	p(lp_1)	Valency angle/lone pair parameter
17	p(val_9)	Valency angle
18	p(val_{10})	Valency angle parameter
19	n.u.	
20	p(pen_2)	Double bond/angle parameter
21	p(pen_3)	Double bond/angle parameter: overcoord
22	p(pen_4)	Double bond/angle parameter: overcoord
23	n.u.	
24	p(tor_2)	Torsion/BO parameter
25	p(tor_3)	Torsion overcoordination
26	p(tor_4)	Torsion overcoordination
27	n.u.	
28	p(cot_2)	Conjugation
29	p(vdW_1)	vdWaals shielding
30	bo_cut	Cutoff for bond order (*100)
31	p(coa_4)	Valency angle conjugation parameter
32	p($ovun_4$)	Overcoordination parameter
33	p($ovun_3$)	Overcoordination parameter
34	p(val_8)	Valency/lone pair parameter
35	n.u.	
36	n.u.	
37	n.u.	
38	gp_{37}	Molecular energy
39	p(coa_3)	Valency angle conjugation parameter

2. ATOM

1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
ro_{sigma}	Val	mass	Rvdw	D_{ij}	gamma	ro(pi)	Val(e)
9	**10**	**11**	**12**	**13**	**14**	**15**	**16**
alfa	gamma(w)	Val(angle)	p($ovun_5$)	n.u.	chiEEM	etaEEM	n.u.
17	**18**	**19**	**20**	**21**	**22**	**23**	**24**

ro(pipi)	p(lp_2)	Heat incr.	p(boc_4)	p(boc_3)	p(boc_5)	n.u.	n.u.
25	**26**	**27**	**28**	**29**	**30**	**31**	**32**
p($ovun_2$)	p(val_3)	n.u.	Val(boc)	p(val_5)	rij_{in}	D_{in}	$alpha_{in}$
33	**34**	**35**	**36**	**37**	**38**	**39**	**40**
lg_1	lg_2						

3. Bond

1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
De(sigma)	De(pi)	De(pipi)	p(be_1)	p(bo_5)	13corr	p(bo_6)	p($ovun_1$)
9	**10**	**11**	**12**	**13**	**14**	**15**	**16**
p(be_2)	p(bo_3)	p(bo_4)	n.u.	p(bo_1)	p(bo_2)	n.u.	n.u.

4. Off-diagonal

1	**2**	**3**	**4**	**5**	**6**	**7**
Dij	RvdW	alfa	ro(sigma)	ro(pi)	ro(pipi)	lg(cij)

5. Angle

1	**2**	**3**	**4**	**5**	**6**	**7**
Thetao,o	p(val_1)	p(val_2)	p(coa_1)	p(val_7)	p(pen_1)	p(val_4)

6. Torsion

1	**2**	**3**	**4**	**5**	**6**	**7**
V_1	V_2	V_3	p(tor_1)	p(cot_1)	n.u	n.u.

7. Hydrogen bond

1	**2**	**3**	**4**
r(hb)	p(hb_1)	p(hb_2)	p(hb_3)

Note: line 5 in atom section and column 7 in off-diagonal section are ONLY used if the low-gradient London dispersion correction is active in ReaxFF. Parameters 30, 31 and 32 in atom section are ONLY needed when inner-wall correction is used in ReaxFF.

n.u=Not Used